

Guanidine, (2-benzothiazolyl)-
2582-07-2 | DTXSID20180474

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 7.33e-01

Global applicability domain: Inside

Local applicability domain index: 4.17e-01

Confidence level: 4.32e-01

Nearest Neighbors from the Training Set

Image not found

2-(1-thiophen-2-ylethylideneamino)guanidine

Measured: 1.05

Predicted: 1.08

Image not found

N-(4-methyl-1,3-thiazol-2-yl)guanidine

Measured: 1.24

Predicted: 9.09e-01

Image not found

2,4-Quinazolinediamine, 5-bromo-

Measured: 1.91

Predicted: 1.36

Image not found

Sulfaguanidine

Measured: -1.22

Predicted: 3.62e-01

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2-Amino-3H-quinazolin-4-one

Measured: 0.6

Predicted: 4.64e-01